

Remarks about the Phase Transitions within the Microcanonical description

L. Velazquez¹ and F. Guzman²

¹*Departamento de Física, Universidad de Pinar del Rio,
Marti 270, Esq. 27 de Noviembre, Pinar del Rio, Cuba*

²*Instituto Superior de Tecnologia y Ciencias Aplicadas,
Quinta de los Molinos, Plaza de la Revolucion, La Habana, Cuba*

(Dated: February 6, 2008)

Abstract

According to the *reparametrization invariance* of the microcanonical ensemble, the only microcanonically relevant phase transitions are those involving an *ergodicity breaking* in the thermodynamic limit: the zero-order phase transitions and the continuous phase transitions. We suggest that the microcanonically relevant phase transitions are not associated directly with topological changes in the configurational space as the *Topological Hypothesis* claims, instead, they could be related with topological changes of certain subset \mathcal{A} of the configurational space in which the system dynamics is effectively trapped in the thermodynamic limit $N \rightarrow \infty$.

PACS numbers: 05.70.-a; 05.20.Gg

INTRODUCTION

Recently, a new characterization of phase transitions has been suggested by Pettini and coworkers [1, 2, 3, 4]. According to the *Topological Hypothesis* proposed by these authors, there should be a close relationship between the existence of a thermodynamic phase transition at the macroscopic level and the existence of *changes in the topological structure* of the configurational space of a generic many-body Hamiltonian system:

$$H(q, p) = \sum_{ij} \frac{1}{2} a^{ij}(q) p_i p_j + V(q). \quad (1)$$

A very important result obtained in this direction was the derivation of the *necessary character* of the topological changes for the existence of a phase transition [1, 2, 3, 4]. The nowadays interest concentrates in searching those *sufficient and necessary conditions* which lead to a topological classification scheme for phase-transitions.

As already shown in many studies [1, 2, 3, 4, 5], most of topological changes in the microscopic level do not provoke a phase transition, apparently, only those strong topological changes. However, Kastner have shown strong evidences about that a criterion based exclusively on topological quantities cannot exist in general [6]. The efforts for establishing the sufficient and necessary relations between topological changes and phase transitions turn to be much more complicated by considering the phenomenon of the ensemble inequivalence. The same author has shown some evidences indicating that such close relation is expected to exist *only* between the topological approach and the microcanonical characterization [7].

We will show in the present Letter that the microcanonical description is characterized by the existence of an internal symmetry: *the reparametrization invariance*. The presence of this symmetry implies a revision of clas-

sification of phase transitions based on the concavity of the Boltzmann entropy [8], as well as the question about the topological origin of the phase transitions by starting from microcanonical basis.

REPARAMETRIZATION INVARIANCE

Universality of the microscopic mechanisms of chaoticity provides a general background for justifying the necessary ergodicity which supports a thermostistical description with microcanonical basis for all those nonintegrable many-body Hamiltonian systems [9]. Thus, the microcanonical ensemble:

$$\hat{\omega}_M(I, N) = \frac{1}{\Omega(I, N)} \delta \langle I - \hat{I}(X) \rangle, \quad (2)$$

is just a *dynamical ensemble* where every macroscopic characterization has a direct mechanical interpretation. Here, X represents a given point of the phase space \mathcal{X} and $\hat{I}(X) = \{\hat{I}^1(X), \hat{I}^2(X), \dots, \hat{I}^n(X)\}$ are all those relevant (analytical) integrals of motion determining the microcanonical description (generally speaking, the total energy, the angular and linear momentum).

The admissible values of the set of integrals of motion $\hat{I}(X)$ could be considered as the "coordinate points" $I = \{I^1, I^2, \dots, I^n\}$ of certain subset \mathcal{R}_I of the n -dimensional Euclidean space \mathcal{R}^n . Each of these points determines certain sub-manifold \mathcal{S}_p of the phase space \mathcal{X} :

$$X \in \mathcal{S}_p \equiv \{X \in \mathcal{X} \mid \forall k \ I^k(X) = I^k\}, \quad (3)$$

in which the system trajectories spread uniformly in accordance with the ergodic character of the microscopic dynamics. Such sub-manifolds defines a partition \mathfrak{S} of the phase space \mathcal{X} in disjoint sub-manifolds:

$$\mathfrak{S} = \left\{ \mathcal{S}_p \subset \mathcal{X} \mid \bigcup_p \mathcal{S}_p = \mathcal{X} ; \mathcal{S}_p \cap \mathcal{S}_q = \emptyset \right\}. \quad (4)$$

Definitions (3) and (4) allow the existence of a bijective map ψ_I between the elements of \mathfrak{S} (sub-manifolds $\mathcal{S}_p \subset \mathcal{X}$) and the elements of \mathcal{R}_I (points $I \in \mathcal{R}^n$):

$$\psi_I : \mathfrak{S} \rightarrow \mathcal{R}_I \equiv \{\forall \mathcal{S}_p \in \mathfrak{S}(\mathcal{X}) \exists I \in \mathcal{R}_I \subset \mathcal{R}^n\}. \quad (5)$$

Thus, the partition \mathfrak{S} has the same topological features of the n -dimensional Euclidean subset \mathcal{R}_I . For this reason \mathfrak{S} will be referred as the *abstract space of the integrals of motions*. We say that the map ψ_I defines the n -dimensional Euclidean *coordinate representation* \mathcal{R}_I of the abstract space \mathfrak{S} .

Let us now to consider another subset $\mathcal{R}_\varphi \subset \mathcal{R}^n$ with the same *diffeomorphic structure* of the subset \mathcal{R}_I and the following diffeomorphic map φ among them:

$$\varphi : \mathcal{R}_I \rightarrow \mathcal{R}_\varphi \equiv \left\{ \forall I \in \mathcal{R}_I \exists \varphi \in \mathcal{R}_\varphi \left| \det \left(\frac{\partial \varphi^j}{\partial I^k} \right) \neq 0 \right. \right\}. \quad (6)$$

We say that the map φ represents a general *reparametrization change* of the microcanonical description since it allows us to introduce another n -dimensional Euclidean coordinate representation \mathcal{R}_φ by considering the bijective map $\psi_\varphi = \psi_I \circ \varphi^{-1}$:

$$\psi_\varphi : \mathfrak{S} \rightarrow \mathcal{R}_\varphi \equiv \{\forall \mathcal{S}_p \in \mathfrak{S} \exists \varphi \in \mathcal{R}_\varphi \subset \mathcal{R}^n\}. \quad (7)$$

The above reparametrization change φ also induces the following reparametrization of the relevant integrals of motion $\varphi_X : \hat{I}(X) \rightarrow \hat{\varphi}(X)$, where:

$$\hat{\varphi}(X) = \left\{ \varphi^1 \langle \hat{I}(X) \rangle, \varphi^2 \langle \hat{I}(X) \rangle, \dots, \varphi^n \langle \hat{I}(X) \rangle \right\}. \quad (8)$$

Since $\hat{I}(X)$ are integrals of motions, every $\varphi^k \langle \hat{I}(X) \rangle \in \hat{\varphi}(X)$ will be also an integral of motion. The bijective character of the reparametrization change $\varphi : \mathcal{R}_I \rightarrow \mathcal{R}_\varphi$ allows us to say that the sets $\hat{\varphi}(X)$ and $\hat{I}(X)$ are *equivalent representations* of the relevant integrals of motion of the microcanonical description because of they generate the same phase space partition \mathfrak{S} (4).

The interesting question is that the microcanonical ensemble is *invariant* under every reparametrization change. Considering the identity:

$$\delta \langle \varphi - \hat{\varphi}(X) \rangle \equiv \left| \frac{\partial \varphi}{\partial I} \right|^{-1} \delta \langle I - \hat{I}(X) \rangle, \quad (9)$$

where $|\partial \varphi / \partial I| \neq 0$ is the Jacobian of the reparametrization change φ , the phase space integration leads to the following transformation rule for the microcanonical partition function:

$$\Omega(\varphi, N) = \left| \frac{\partial \varphi}{\partial I} \right|^{-1} \Omega(I, N), \quad (10)$$

leading in this way to the reparametrization invariance of the microcanonical distribution function:

$$\frac{1}{\Omega(\varphi, N)} \delta \langle \varphi - \hat{\varphi}(X) \rangle \equiv \frac{1}{\Omega(I, N)} \delta \langle I - \hat{I}(X) \rangle. \quad (11)$$

A corollary of the identity (11) is that the Physics derived from the microcanonical description is reparametrization invariant since the expectation values of every macroscopic observable $\hat{O}(X)$ obtained from the microcanonical distribution function $\hat{\omega}_M(X)$ exhibits this kind of symmetry:

$$\bar{O} = \int \hat{O}(X) \hat{\omega}_M(X) dX \Rightarrow \bar{O}(\varphi, N) = \bar{O}(I, N). \quad (12)$$

The reparametrization invariance does not introduce anything new in the macroscopic description of a given system, except the possibility of describing the microcanonical macroscopic state by using any coordinate representation of the abstract space \mathfrak{S} , a situation analogue to the possibility of describing the physical space \mathcal{R}^3 by using a Cartesian coordinates (x, y, z) or a spherical coordinates (r, θ, φ) . Thus, we can develop a geometrical formulation of Thermostatistics within the microcanonical ensemble.

The microcanonical partition function allows us to introduce an invariant measure $d\mu = \Omega dI$ for the abstract space \mathfrak{S} , leading in this way to an invariant definition of the Boltzmann entropy $S_B = \ln W$, where $W = \int_{\Sigma_\alpha} d\mu$ characterizes certain *coarse grained* partition $\{\Sigma_\alpha | \bigcup_\alpha \Sigma_\alpha = \mathfrak{S}\}$. In the thermodynamic limit $N \rightarrow \infty$ the coarsened nature of the Boltzmann entropy can be disregarded and taken as a scalar function defined on the space \mathfrak{S} .

MICROCANONICAL PHASE TRANSITIONS

The present proposal comes from by arising the above reparametrization invariance to a fundamental status within the microcanonical description. In the sake of simplicity, let us consider a Hamiltonian system with a microscopic dynamics driven by short-range forces, so that, it becomes extensive in the thermodynamic limit. Let us suppose also that its microcanonical description is determined from the consideration of only one integral of motion: the total energy E . Among all different reparametrizations of the total energy E which can be taken into account, we shall limit only to the following generic form $\Theta = N\varphi(E/N)$, where N represents the system size and $\varphi(\varepsilon)$, an analytical bijective function of the energy per particle $\varepsilon = E/N$. Obviously, the quantity Θ represents an integral of motion of the microscopic dynamics which has the advantage of preserving the same extensive character of the energy in the thermodynamic limit. Hereafter, the function $\varepsilon(\varphi)$ represents the inverse of the function $\varphi(\varepsilon)$.

Taking into account the dynamical origin of the microcanonical description, a phase transition within this ensemble should be the macroscopic manifestation of certain sudden change in the microscopic level which manifests itself as a mathematical anomaly of the Boltz-

mann entropy. Since the entropy is usually an analytical function in a finite system, the most important mathematical anomalies of the entropy per particle $s(\varphi) = S_B \langle \varepsilon(\varphi) N, N \rangle / N$ are **(A)** the existence of regions where this function is not locally concave (convex down), $\partial^2 s(\varphi) / \partial \varphi^2 \geq 0$, as well as **(B)** every loss of analyticity in the thermodynamic limit $N \rightarrow \infty$.

The non concavity of the entropy is usually related with the phenomenon of ensemble inequivalence between the microcanonical description and the one performed by using the Gibbs canonical ensemble, which is associated with the occurrence of the first order phase transitions. However, the behavior **A** represents an anomaly within the canonical description because of there is nothing anomalous within the microcanonical ensemble: these regions represent microcanonical thermodynamic states with a negative heat capacity, which can not be accessed within the canonical ensemble when the thermodynamic limit is invoked [8]. A negative heat capacity in systems with short-range interactions outside the thermodynamic limit is identify with the existence of a non-vanishing interphase surface tension [8]. While this phenomenon disappears in these systems with the imposition of the thermodynamic limit, it survives in systems with long-range interactions, i.e. the astrophysical systems [10, 11]. Although they are non-homogeneous, a negative heat can not be always identified with the existence of interphase boundaries, which can be verified by reexamining the Antonov isothermal model [10].

The reader can notice by considering the microcanonical reparametrization invariance that the convex up or down character of any scalar function is *ambiguous*: it depends on the coordinate representation used for describe it. Let us see a trivial example. Let s be a positive real map defined on a seminfinte Euclidean line \mathcal{R}_1 , $s : \mathcal{R}_1 \rightarrow \mathcal{R}^+$, which is given by the concave function $s(x) = \sqrt{x}$ in the coordinate representation \mathcal{R}_x of \mathcal{R}_1 (where $x > 0$). Let φ be a reparametrization change $\varphi : \mathcal{R}_x \rightarrow \mathcal{R}_y$ given by $y = \varphi(x) = x^{\frac{1}{2}}$ (which is evidently a bijective map). The map s in the new representation \mathcal{R}_y is given by the function $s(y) = y^2$ (where $y > 0$), which clearly is a convex function in this coordinate representation of the domain \mathcal{R}_1 .

Since the convexity of the Boltzmann entropy depends crucially on the reparametrization, the ensemble inequivalence between the microcanonical description and the one performed by using the following *generalization* of the Gibbs canonical ensemble:

$$\hat{\omega}_c(\eta, N) = \frac{1}{Z(\eta, N)} \exp \langle -\eta \Theta \rangle \quad (13)$$

depends also on the reparametrization $\Theta = N\varphi(E/N)$. Such noninvariance of the ensemble inequivalence follows from the fact that the distribution function (13) does not obey the original reparametrization invariance since this ensemble does not describe an *isolate* Hamiltonian sys-

tem: the coordinate representation Θ used in the canonical description has been determined from certain external constrains which has been imposed to the interest system. This idea is very easy to understand by analyzing the case of the extensive systems: the canonical ensemble $\omega_{BG} = Z^{-1}(\beta, N) \exp(-\beta H_N)$ is experimentally implemented by putting the interest system in thermal contact with a heat bath. This experimental arrangement keeps fixed not only the system temperature $T = \beta^{-1}$, but also the coordinate representation by using the system total energy, $\Theta \equiv E$. An arbitrary reparametrization change $E \rightarrow \Theta$ within the canonical ensemble (13) is physically implemented by considering another experimental arrangement which keeps fixed the canonical parameter $\eta = \partial s(\varphi) / \partial \varphi$. The possibility of using different reparametrizations Θ in the canonical distribution function allows us to avoid the ensemble inequivalence in those thermodynamic states with a negative heat capacity, a feature particularly useful for enhancing the possibilities of some general Monte Carlo methods inspired on the Statistical Mechanics. This idea was applied in ref.[12] to improve the well-known Metropolis importance sampling algorithm [13], which is usually unable to describe the thermodynamical states with a negative heat capacity.

Although paradoxical, the identification of the first order phase transitions with the ensemble inequivalence allows us to claim that this kind of phase transitions are not microcanonically relevant because of they are irrelevant from the dynamical viewpoint. Contrary, it is very easy to verify that every loss of analyticity of the microcanonical entropy in the thermodynamic limit appears without mattering about the analytical function $\varphi(\varepsilon)$ used in the reparametrization Θ . Thus, the mathematical anomaly **B** is compatible with the reparametrization invariance of the microcanonical ensemble, and it is apparently the macroscopic manifestation of a sudden change in the behavior of the microscopic dynamics of the system. An reexamination of the available experimental and theoretical results suggests us a direct connection of anomaly **B** with the occurrence of an *ergodicity breaking*. Ergodicity breaking takes place when the time averages and the ensemble averages of certain macroscopic observables can not be identified due to the microscopic dynamics is effectively trapped in different subsets of the configurational or phase space during the imposition of the thermodynamic limit $N \rightarrow \infty$ [14]. Let us see two examples.

It is well-known that ensemble equivalence holds during the *continuous phase transitions* in systems with short-range interactions, but the heat capacity $c(\varepsilon) = -\beta^2(\varepsilon) / \kappa(\varepsilon)$ diverges at the critical energy ε_c in the thermodynamic limit where $\kappa(\varepsilon_c) = 0$, being $\beta = \partial s(\varepsilon) / \partial \varepsilon$ and $\kappa(\varepsilon) = \partial^2 s(\varepsilon) / \partial \varepsilon^2$. It is not difficult to show by using the Taylor power series expansion of the caloric curve $\beta(\varepsilon)$ that the analyticity of the entropy $s(\varepsilon)$ at the critical energy is unable to explain the existence of

nontrivial critical exponent α in the heat capacity close to the critical inverse temperature $\beta_c = \beta(\varepsilon_c)$:

$$c(\beta) \simeq \begin{cases} A^- / (\beta_c - \beta)^\alpha & \text{if } \beta < \beta_c, \\ A^+ / (\beta - \beta_c)^\alpha & \text{if } \beta > \beta_c, \end{cases} \quad (14)$$

with a universal ratio $A^-/A^+ \neq 1$ [14]. This non-analyticity of the entropy in the thermodynamic limit is clearly associated with the occurrence of an ergodicity breaking during the continuous phase transitions as a consequence of an underlying symmetry breaking.

Another evidence of such connection is during the occurrence of the called *zero-order phase transitions* in systems with long-range interactions [11]. This anomaly manifests itself as a discontinuity in the first derivative of the entropy, which represents the existence of equiprobable metastable states with different temperatures at the same total energy. Depending from the initial conditions, only one of these metastable configurations will be given in practice when $N \rightarrow \infty$.

Apparently, every lost of analyticity of the entropy in the thermodynamic limit can be associated with the existence of several metastable states (sub-manifolds in the configurational space) in which the system dynamics can be effectively trapped in the thermodynamic limit: While all these metastable states in the continuous phase transitions are related by an internal symmetry of the microscopic dynamics, the metastable states in the zero-order phase transitions are essentially different (not related by an internal symmetry). These are the only phase transitions which are relevant anomalies within the microcanonical ensemble. They have an evident dynamical origin which can be associated with mathematical anomalies of the entropy compatible with the reparametrization invariance of the microcanonical ensemble.

Does every phase transition have a Topological origin? We think that the answer to this question is negative due to the only phase transitions which are dynamically relevant in an isolate nonintegrable many-body Hamiltonian system are those involving an ergodicity breaking in the microscopic picture. While a classification scheme of the phase transitions based exclusively on the topology of configurational space cannot exist in general [6], it is not difficult to understand that an ergodicity breaking in the thermodynamic limit always involves certain *effective topological change* in the configurational space.

Let us consider a classical 2-dimensional ferromagnetic model system with a microscopic magnetization density \mathbf{m} given by $\mathbf{m}[\theta] = N^{-1} \sum_i (\cos \theta_i, \sin \theta_i)$, whose Hamiltonian exhibits a $U(1)$ symmetry, and where the configurational space is the N -dimensional tori $\mathcal{C} = \{0 < \theta_i \leq 2\pi; i = 1, \dots, N\}$. The equilibrium distribution function of the modulus of the magnetization density $m = |\mathbf{m}|$ when N is large enough exhibits a very sharp Gaussian profile around the certain average value $m_0(\varepsilon)$ which depends on the energy per particle ε , with a dispersion decreasing as $\sigma_m \propto 1/\sqrt{N}$. Thus, the imposition

of the thermodynamic limit leads to an *effective trapping* of the microscopic dynamics in the following subset of the configurational space:

$$\mathcal{A}(\varepsilon) = \{\theta \in \mathcal{C} \mid |\mathbf{m}[\theta]| = m_0(\varepsilon)\}. \quad (15)$$

Since the average magnetization density vanishes identically in the paramagnetic phase (with ε greater than certain critical energy ε_c), the dimension of the subset $\mathcal{A}(\varepsilon)$ is $\dim \langle \mathcal{A}(\varepsilon) \rangle = N - 2$, and its codimension $C \langle \mathcal{A}(\varepsilon) \rangle = \dim \mathcal{C} - \dim \langle \mathcal{A}(\varepsilon) \rangle = 2$ is topological invariant in the thermodynamic limit $N \rightarrow \infty$. In the ferromagnetic phase with $\varepsilon < \varepsilon_c$, the system exhibits a spontaneous magnetization with an arbitrary orientation due to the $U(1)$ symmetry. The dimension of the subset $\mathcal{A}(\varepsilon)$ is now $\dim \langle \mathcal{A}(\varepsilon) \rangle = N - 1$, and its codimension is given by $C \langle \mathcal{A}(\varepsilon) \rangle = \dim \mathcal{C} - \dim \langle \mathcal{A}(\varepsilon) \rangle = 1$, which is also topological invariant when $N \rightarrow \infty$. Thus, during the continuous phase transition there is a topological change of the codimension $C \langle \mathcal{A}(\varepsilon) \rangle$ of the subset $\mathcal{A}(\varepsilon)$.

This example suggests us that the microcanonically relevant phase transitions are not directly associated with topological changes in the configurational space as the *Topological Hypothesis* claims [1, 2, 3, 4], instead, we think that they could be related with certain topological change of subset \mathcal{A} of the configurational space in which the system dynamics is effectively trapped in the thermodynamic limit $N \rightarrow \infty$.

-
- [1] L. Caiani, L. Casetti, C. Clementi, and M. Pettini, Phys. Rev. Lett. **79** (1997) 4361.
 - [2] R. Franzosi, M. Pettini, and L. Spinelli, Phys. Rev. Lett. **84** (2000) 2774.
 - [3] L. Casetti, M. Pettini, and E.G.D. Cohen, Phys. Rep. **337** (2000) 237.
 - [4] R. Franzosi and M. Pettini, Phys. Rev. Lett. **92** (2004) 060601.
 - [5] P. Grinza and A. Mossa, Phys. Rev. Lett. **92** (2004) 158102 and references therein.
 - [6] M. Kastner, Phys. Rev. Lett. **93** (2004) 150601
 - [7] M. Kastner, Physica A **359** (2006) 447.
 - [8] D.H.E. Gross, *Microcanonical thermodynamics: Phase transitions in Small systems, 66 Lectures Notes in Physics*, (World scientific, Singapore, 2001).
 - [9] G. Gallavotti, E.G.D. Cohen, Phys. Rev. Lett. **74** (1995) 2694 ; J. Stat. Phys. **80** (1995) 931.
 - [10] V.A. Antonov, Vest. leningr. gos. Univ. **7** (1962) 135.
 - [11] P.H. Chavanis, Phys. Rev. E **65** (2002) 056123.
 - [12] L. Velazquez and J. C. Castro Palacio, *Metropolis Monte Carlo algorithm based on reparametrization invariance*, e-print (2006) [cond-mat/0606727].
 - [13] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, J. Chem. Phys. **21** (1953) 1087.
 - [14] N. Goldenfeld, *Lectures on phase transitions and critical phenomena*, Frontiers in physics 85, (Perseus Books Publishing, L.L.C., 1992).